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TITLE: Proceedings IEEE Lester Eastman Conference on High Performance Devices at University of Delaware, Newark, Delaware, August 6, 7, and 8. 2002

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Monte Carlo Simulation of InGaAs/InAlAs HEMTs with a Quantum Correction Potential

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Abstract

In Monte Carlo simulation of high electron mobility transistors (HEMTs), how to position the source and drain contacts will significantly affect the drain current. Unlike many Monte Carlo (MC) simulations of HEMTs in the past, in this work, the source and drain contacts are placed on the top of the caps as in the real device instead of on the side adjacent to the channel. In addition, to take quantum effects into consideration, the effective potential approach of quantum correction has been incorporated into our MC simulator. We have found that the simulated drain current is substantially increased compared to that of using the classical potential.

I. Introduction

HEMTs have been extensively used in high-frequency applications, such as high power and low noise amplifiers. Due to expensive cost of processing HEMTs, it is desirable to predict their performance by simulation and by doing so to improve their design parameters. However, most existing simulators which use drift-diffusion (DD) or hydrodynamic (HD) model are not able to simulate complicated heterostructures with sufficient accuracy. Although some HD simulators [1][2] are capable of producing results which agree with the experimental data well, often a silicon-like mobility model is used in the simulation and extensive parameter adjustment is required. The alternate simulation tool is the ensemble Monte Carlo (EMC) method which does not require assumption of the mobility model. This approach is employed in this work for the simulation of HEMTs.

In most reported Monte Carlo (MC) simulations of HEMTs [3][4], the drain and source contacts are extended down to the channel as shown in Fig.1 (a). In this case, most electrons drift from the source end of the channel to the drain end and are collected by the extended drain contact without crossing the heterojunction, as indicated by the dotted line. However, in a real device, the Ohmic contact is placed on the top of the cap layers as shown in Fig. 1(b) where the typical electron flow path is indicated by the dotted line. Our two

dimensional self-consistent MC simulation shows that if the top contacts are used, the drain current I_D predicted by the MC method is much smaller than the experimentally measured data. This observation is also confirmed by Simlinger et al. using the DD model [5]. The

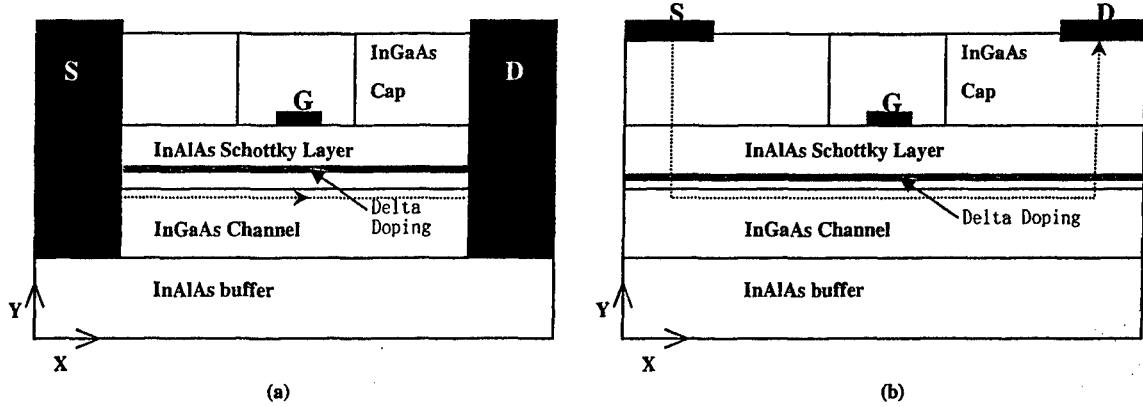


Fig. 1 The structure of HEMT (a) with contacts extended into the channel. (b) with contacts on top of the caps.

main reason for this is that the particle injection scheme at the contacts plays an important role in the simulation. We have found that if particles are injected into the device in order to maintain the charge neutrality near the Ohmic contacts, use of an injection scheme according to the weighted Maxwellian distribution [6] rather than the hemi-Maxwellian distribution [7] will increase the drain current by approximately 20 percent. In addition, in the classical transport model, only the thermionic emission is considered for the real space transfer. It is well known that the quantization effect in the channel and the tunneling effect across the Schottky layer must be taken into account for realistic HEMT simulation. This is usually implemented by solving the Schrödinger equation coupled with the Poisson equation. However, this approach is very time consuming, especially for self-consistent ensemble MC simulation. Therefore, some alternative methods are adopted by many researchers, such as the field assisted barrier lowering [1][5] and the non-local Schottky contact model [2].

II The Effective Potential Method of Quantum Correction

In recent years, the effective potential (EP) approach has been established as a viable alternative to the solution of Schrödinger equation for incorporating certain quantum effects. In the original paper by Feynman and Kleinert [8], the EP was used to study bounded carriers in a symmetric anharmonic oscillator and a double-well potential. Subsequently the EP approach has been applied to semiconductor devices [9][10][11][12], which has advantage of easy numerical implementation and almost guaranteed convergence. The EP model is based on the following integral transformation from the classical potential (CP), $V(x)$, to the EP, $V_{eff}(x)$ [8]:

$$V_{eff} = \frac{1}{\sqrt{2\pi}a} \int_{-\infty}^{\infty} V(x+\xi) \exp\left(-\frac{\xi^2}{2a^2}\right) d\xi. \quad (1)$$

The idea of proposing the EP for device simulation originates in part from the consideration of the finite-size effect of charge carriers [8][13]. When the electric potential produced by a point charge (represented by a delta function) is replaced by a finite-size wave packet (represented by a Gaussian function), the CP is smoothed out and it results in an EP as given by (1). The integral form of V_{eff} as given in (1) suggests that V_{eff} is a convolution of $V(x)$ with a Gaussian function with the standard deviation a .

In this work, we modify the EMC simulation code to account for the quantum effects by smoothing the classical potential V to obtain the effective potential V_{eff} by (1).

III Simulation Experiments

The structure of a HEMT we simulated is as shown in Fig.1 (b). The gate length is 150 nm, the cap doping is 10^{18} cm^{-3} and the δ -doping is $1.5 \times 10^{19} \text{ cm}^{-3}$. The thickness of the channel is 20 nm and that of the Schottky layer is 18 nm. The length of the recess is 0.5 μm and the total length of the device is 3.5 μm . A uniform rectangular mesh is used to avoid the self-force effect [14] and 40,000 particles are used in the simulation. Our EMC simulator adopts a non-parabolic 3-valley energy band structure and uses a synchronous scheme [14] with a constant time step dt equal to 2fs. We advance the particle's position by the equation (taking the y -direction as example)

$$y^{(i+1)} = y^{(i)} + \frac{1}{2}(v_i + v_f) \cdot \Delta t \quad (2)$$

rather than by the one suggested in [3]:

$$y^{(i+1)} = y^{(i)} + v_i \cdot \Delta t + \frac{1}{2} \frac{qE_y}{m^*} (\Delta t)^2 \quad (3)$$

where, v_i and v_f are the y -components of initial velocity and final velocity, respectively, and E_y is the y -component of the electric field. When a particle crosses a hetero-interface, the time step dt is split into $dt1$ and $dt2$ which are respectively the times the particle spends during this time step before and after crossing the hetero-interface. The time intervals $dt1$ and $dt2$ are solved by (2) implicitly by an iteration scheme rather than by (3) explicitly. We have found that the former approach makes the simulation result less sensitive to the size of time step when the top drain and source contacts are used and when the electric field is very high.

At the beginning of each time step dt , the Poisson equation is solved and the effective potential V_{eff} is evaluated by (1). We choose the parameter a in (1) to be 1.92 nm, three times the theoretical value

$$a_0 = \hbar / \sqrt{8mk_B T} \quad (4)$$

which is often treated as an adjusting parameter. The effective mass m^* of the Schottky layer material is $0.083m$; thus if we substitute m by m^* into (4), we will obtain a value roughly three times a_0 . The force exerted on the particles is then calculated by the effective potential V_{eff} rather than by the classical potential. Only carriers in the Gamma valley are subject to the effective potential in our simulation since we consider that most of the carriers reside in the Gamma valley.

In Fig.2, we show the conduction band edge obtained from the simulation under the bias condition of $V_g = -0.2\text{V}$ and $V_d = 1.0\text{V}$. From Fig.2 (a) and (b) we can see that the

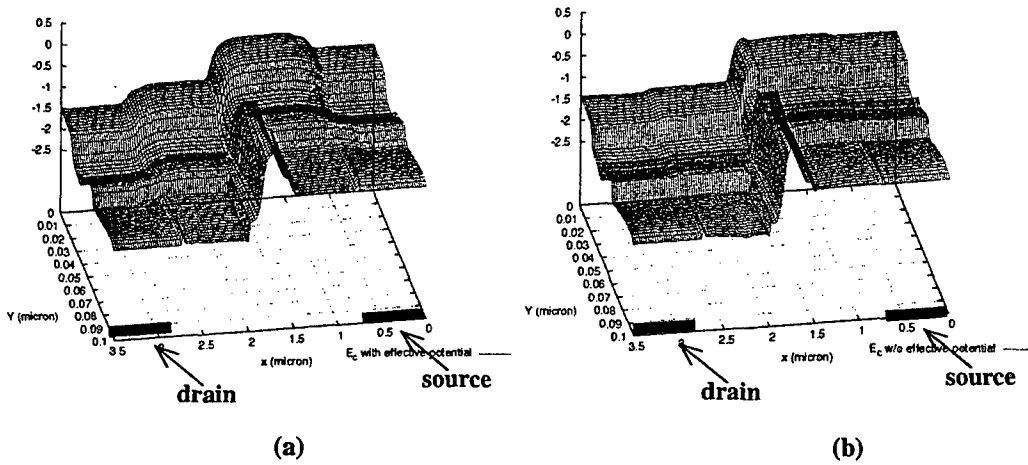


Fig.2 Conduction band edge for applied bias $V_g = -0.2\text{V}$ and $V_d = 1.0\text{V}$
 (a) with the effective potential (b) without the effective potential.

abrupt conduction band discontinuities have been smoothed out by the EP. Fig.3, Fig.5 and Fig.7 show the conduction band edge along the y -direction on the source side, under the gate and on the drain side, respectively. We find that the band edge in the channel is lifted and the barrier between the channel and the cap is lowered. Therefore more carriers can go over the Schottky layer and flow into the drain cap. In Fig.4, Fig.6 and Fig.8, we plot the corresponding electron density along the same line in the y -direction. A significant increase of electron density in Schottky layer can be observed. This means that the tunneling effect has been effectively included in the EP. In addition, the conduction band edge in the cap layer (see Fig. 3) with the EP becomes flat compared to that with the classical result. With the EP, it is easier for the carriers to move to the top of the cap layer and be collected by the drain contact. The output characteristic is shown in Fig.9. As expected, under the same bias condition, the drain current is increased by about 20 percent compared to that of the classical result.

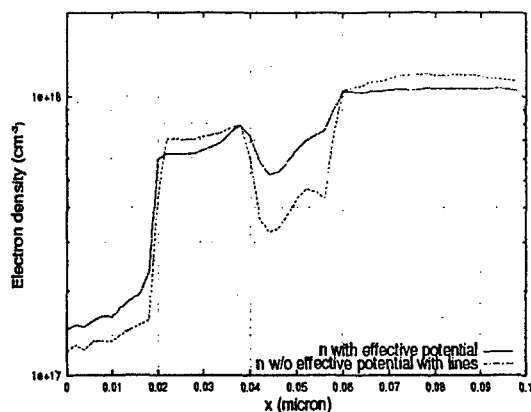


Fig.3 Conduction band edge along Y direction at the source side.

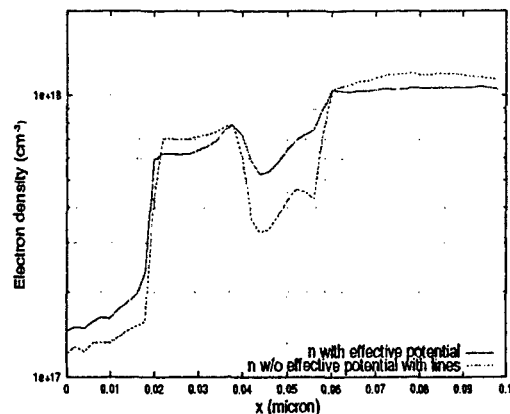


Fig.4 Electron density along Y direction at the source side.

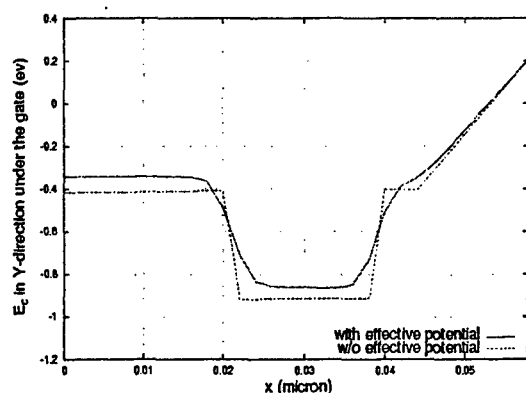


Fig.5 Conduction band edge along Y direction under the gate.

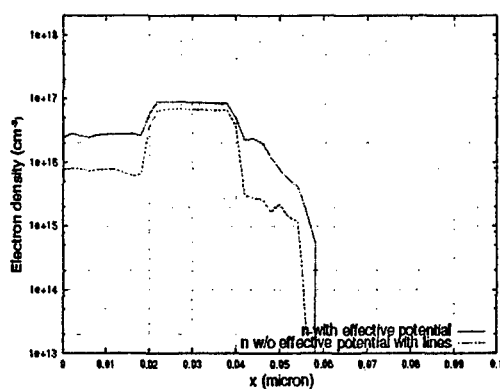


Fig.6 Electron density along Y direction under the gate

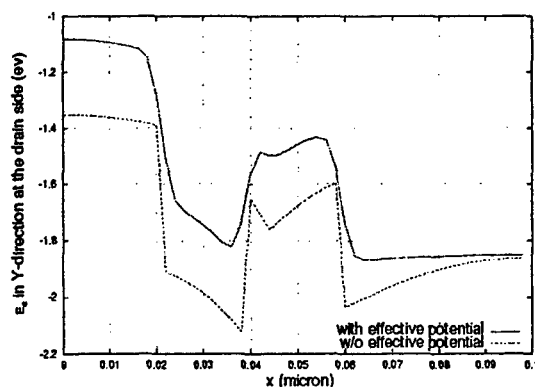


Fig.7 Conduction band edge along Y direction at the drain side.

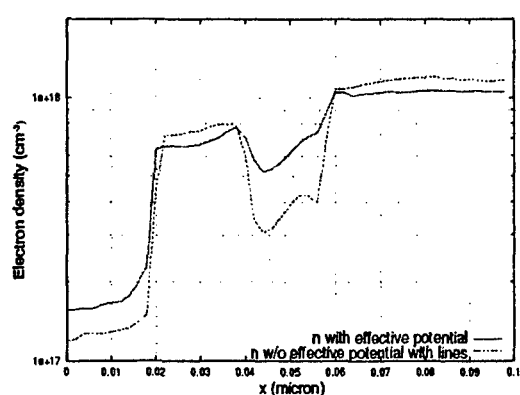


Fig.8 Electron density along Y direction at the drain side.

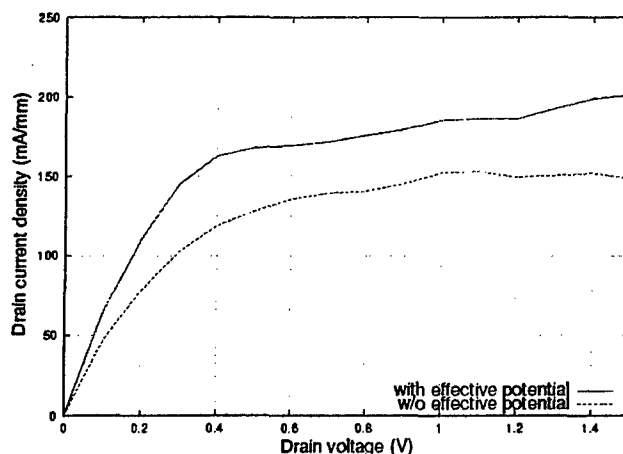


Fig. 9 Drain current vs. Drain voltage under the bias condition $V_G = -0.2V$ and $V_D = 1.0V$.

III Conclusion

In summary, when the contact is placed on top of the cap layer, the classical transport scheme gives very low I_D because the carriers cannot easily get out from the channel to the Schottky layer and be collected by the drain. However, when the effective potential is utilized to incorporate the quantum effects, the result is substantially improved and is much closer to the experimental data. We find that the particle injection scheme at Ohmic contacts also affects the drain current, and we expect a even larger current if a weighted displaced Maxwellian distribution [15] is used for the particle injection.

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